

Argonne National Laboratory

**1559/RE: A CODE TO COMPUTE
RESONANCE INTEGRALS IN MIXTURES**

by

Charles N. Kelber

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ANL-6709
Mathematics and
Computers
(TID-4500, 20th Ed.)
AEC Research and
Development Report

SUMMARY

I. EQUATIONS ARGONNE NATIONAL LABORATORY
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Argonne, Illinois

II. METHOD OF SOLUTION - CROSS SECTIONS

IV. INPUT PREPARATION

V. OUTPUT

VI. EARLY RESULTS AND PROGRAM OF FUTURE WORK

1559/RE: A CODE TO COMPUTE
BIBLIOGRAPHY RESONANCE INTEGRALS IN MIXTURES

ACKNOWLEDGMENTS by

APPENDIX A - THE AUTHOR Charles N. Kelber

Reactor Engineering Division

May 1963

Operated by The University of Chicago
under
Contract W-31-109-eng-38
with the
U. S. Atomic Energy Commission

TABLE OF CONTENTS

	<u>Page</u>
SUMMARY	4
I. EQUATIONS SOLVED	4
II. METHOD OF SOLUTION - COLLISION DENSITY	6
III. METHOD OF SOLUTION - CROSS SECTIONS	7
IV. INPUT PREPARATION	8
V. OUTPUT	11
VI. EARLY RESULTS AND PROGRAM OF FUTURE WORK	11
BIBLIOGRAPHY	14
ACKNOWLEDGEMENT	14
APPENDIX A - Typical Fortran Listing for 1559/RE	15

LIST OF FIGURES

<u>No.</u>	<u>Title</u>	<u>Page</u>
I.	Flux Per Unit Lethargy in an H/U Mixture	12
II.	Effective Resonance Integrals of U ²³⁵ in H/U = 1 Mixture; and α of U ²³⁵	13

LIST OF TABLES

I.	Resonance Parameters	10
II.	Resonance Integral of Dilute Gold	12

1. RESONANCE APPROXIMATION

The collision density is given by an integral equation for elastic scattering by atoms of all species.⁽¹⁾ In this report we assume all atoms are heavy or light (moderator) and in the moderator terms we use the narrow-resonance approximation; we replace the collision density by its asymptotic form. In using the code presented here, the moderation constants should be adjusted to give the correct asymptotic form.

RESINT solves the equations

$$\Gamma(U) = \frac{1}{\pi} \int_{E_L}^{\infty} \Gamma(U') A(U') dU' + \frac{\lambda_m}{E(U)} \quad (1)$$

and

$$\text{RESINT}(U, E_L) \approx \int_{E(E_L)}^{E(E_U)} \Gamma(U) E(U) \frac{dU}{dt} \quad (2)$$

The term RESINT is the resonance integral times the atomic density. Both

$\Gamma(U)$ = the collision density at lethargy U , per unit energy

E_U = upper energy limit (ev)

E_L = lower energy limit (ev)

$A(U)$ = e^{-NU}

λ_m = "moderator" scattering cross section

λ = heavy atom scattering term; $\lambda = 4A/(A+1)$

α = maximum logarithmic decrement in energy from nuclear scattering, in units of lethargy.

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SUMMARY

1559/RE is an experimental IBM-704 code in FORTRAN language to compute the resonance integrals of isotopes in mixtures in the presence of hydrogenic moderation. There may be up to four isotopes, each with no more than 75 resolved resonance levels. Doppler broadening and interference scattering are included. No estimate is made of contributions from unresolved resonances. Typical running times are 30 min (with no Doppler broadening) to 90 min (with Doppler broadening) for problems involving 67 levels and unit lethargy widths.

I. EQUATIONS SOLVED

The collision density is given by an integral equation involving scattering by atoms of all species.⁽¹⁾ In this report we assume all atoms are heavy or light (moderator) and in the moderator terms we use the narrow-resonance approximation; we replace the collision density by its asymptotic form. In using the code presented here, the moderator constants should be adjusted to give the correct asymptotic form.

1559/RE solves the equations

$$F(U) = \frac{1}{\alpha} \int_{U-\Delta}^U F(U') A(U') dU' + \frac{\Sigma_m}{E(U)} \quad (1)$$

and

$$RESINT(i,j) = N_i \int_{U(E_U)}^{U(E_L)} F(U) E(U) \frac{\sigma_{ji}}{\Sigma_t} du \quad . \quad (2)$$

The term RESINT is the resonance integral times the atomic density. Also,

$F(U)$ = the collision density at lethargy U , per unit energy

E_U = upper energy limit (ev)

E_L = lower energy limit (ev)

$E(U) = e^{-U} E_U$

Σ_m = "moderator" scattering cross section

α = heavy atom scattering term; $\alpha = 4A/(A + 1)^2$

Δ = maximum logarithmic decrement in energy from heavy atom scattering, in units of lethargy.

N_i = number of atoms of isotope i per barn-cm

σ_{ji} = absorption ($j = a$) or fission ($j = f$) cross section of isotope i at energy $E(U)$

$A(U)$ = heavy atom scattering cross section divided by the total cross section.

For each isotope the cross sections are found from:

resonance scattering:

$$\sigma_s = \sum_{K=1}^J \left(\frac{\sigma_{oK} \Gamma_{nK}}{\Gamma_K} \psi_K(E) + \sqrt{\sigma_{pt} \sigma_{okg} \Gamma_{nK} / \Gamma_K} \chi_K(E) \right) ; \quad (3)$$

absorption:

$$\sigma_a = \sum_{K=J}^J \left(\sqrt{\frac{|E_K|}{E}} \frac{(\Gamma_{\gamma K} + \Gamma_{fK})}{\Gamma_K} \sigma_{oK} \psi_K(E) \right) ; \quad (4)$$

fission:

$$\sigma_f = \sum_{K=1}^J \left(\sqrt{\frac{|E_K|}{E}} \frac{\Gamma_{fK}}{\Gamma_K} \sigma_{ok} \psi_K(E) \right) . \quad (5)$$

The various symbols have their usual meanings; in particular,

σ_{pt} = potential scattering of isotope i

σ_{ok} = $(2.62 \times 10^6)g \Gamma_{nK} / (|E_K| \Gamma_K)$

g = statistical weight (assumed constant for all levels of isotope i)

Γ_{nK} = neutron width of resonance K (ev)

E_K = energy of K^{th} resonance (ev)

Γ_K = total width of K^{th} resonance (ev)

Γ_{fK} = fission width of K^{th} resonance (ev)

$\Gamma_{\gamma K}$ = gamma width of K^{th} resonance (ev)

The functions $\psi_K(E)$ and $\chi_K(E)$ are the familiar Doppler-broadened line shapes:

$$\psi(\zeta, x) = \frac{\zeta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\zeta^2(x-y)^2/4}}{1+y^2} dy ; \quad (6)$$

*A_J is a variable, not A times J.

$$\chi(\zeta, x) = \frac{\zeta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} 2y \frac{e^{-\zeta^2(x-y)^2/4} dy}{1+y^2} ; \quad (7)$$

$$\zeta = \left(\frac{A_i \Gamma_K^2}{4E_k T} \right)^{1/2} ; \quad x = \frac{2}{\Gamma_K} (E - E_K) ,$$

where

A_i = isotope mass (amu)

kT = material temperature, ev.

If the temperature kT is exactly 0, the subroutine which generates ψ and χ is not used; instead, $\psi = 1/(1+x^2)$, and $\chi = 2x/(1+x^2)$ are used. The parameters α and $\Delta = \ln[1/(1-\alpha)]$ were not made isotope dependent since 1559/RE is an experimental code designed largely to evaluate the interference effects between similar isotopes. Since we expect to investigate situations where the heavy atom scattering is largely from atoms of mass A , say, we usually take $\alpha = 4A/(A+1)^2$. It is not conceptually difficult to make α and Δ isotope dependent and remove this source of error; the additional programming complication, however, is sufficient to cause this change to be put off to the future.

II. METHOD OF SOLUTION - COLLISION DENSITY

Equations (1) and (2) are solved by trapezoidal integration, the asymptotic solution $F = (\Sigma p_t + \Sigma m)/E$ being used to get started. This method has been frequently used before [see, for example, Nordheim(1)].

A fixed lethargy interval is used during the entire integration scheme. The interval is given by $D = \Delta/N$ (see Eq. 2), where N is input information. Values of N between 25 and 100 are recommended. If N is greater than 100, storage allocations are exceeded and the program causes the machine to print the input error: "N OUT OF RANGE" and proceeds to the next problem.

The integration is carried out over $10N$ steps. Then the upper energy is reset and the integration resumed until the lower energy is less than EL (input). The actual equations solved for the collision density are*

$$AJ_i = AJ_{i-1} - \frac{0.5}{\alpha} (F_{i-N-1} A_{i-N-1} + F_{i-N} A_{i-N}) + F_{i-1} \frac{A_{i-1}}{\alpha} \quad (8)$$

and

$$F_i = [D AJ_i + (\Sigma m/E_i)] / \left(1 - 0.5 D \frac{A_i}{\alpha} \right) , \quad (9)$$

as suggested by Nordheim.(1)

*AJ is a variable, not A times J.

The $N+1$ values necessary to get the set (8,9) started are obtained initially from the asymptotic solution

$$F_i = (\Sigma_{pt} + \Sigma_m)/E_i \quad , \quad \text{for } E_i = E_U e^{(N+1-i)D} \quad , \\ i=1, \dots, N+1 \quad . \quad (10)$$

After the completion of $10N$ lethargy steps, the last $N+1$ values of collision density and the auxiliary quantities AJ_i are stored (on tape 2) and the process restarted, with the information now on tape 2 used to get the set (8,9) going.

A quantity printed out under the misnomer "flux" and equal to $E_i F_i$ is also calculated and is used in getting the resonance integrals (Eq. 2) by trapezoidal integration, using the lethargy step, D . The actual flux per unit lethargy is equal to the printed quantity divided by the total cross section.

III. METHOD OF SOLUTION - CROSS SECTIONS

The sums 3, 4, and 5 are evaluated directly at each energy. At temperature 0, the analytic representations $\psi = 1/(1+x^2)$ and $\chi = 2x/(1+x^2)$ are used for the line shapes.

For temperatures greater than zero, the functions $\psi_K(E)$ and $\chi_K(E)$ are calculated by use of the W subroutine. The W subroutine was written by O'Shea and Thacher(2) for the express purpose of computing resonance line shapes.

The function actually computed is the complex probability integral $W(z)$ defined by

$$W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t} dt \quad . \quad (11)$$

Setting

$$z = \frac{\zeta x}{2} + i \frac{\xi}{2} \quad ,$$

we obtain

$$\psi(\zeta, x) = \frac{\zeta \sqrt{\pi}}{2} R_e W \quad ; \quad \chi(\zeta, x) = \zeta \sqrt{\pi} I_m W$$

(see Eq. 6 and 7). The probability integral $W(z)$ is computed by use of continued fractions:

$$W(z) = e^{-z^2} + \frac{2iz\nu}{\sqrt{\pi}} \left[\frac{1}{\nu - 1/3 +} \frac{2/45}{\nu + 1/21 +} \dots \frac{2r(2r-1)}{(4r-3)(4r+1)(4r-1)^2} \dots \right] \dots ;$$

$$\nu = -1/(2z^2) \quad (12a)$$

In the asymptotic form,

$$W(z) = \frac{2iz}{\sqrt{\pi}} \left[\frac{1}{\nu-1} - \frac{2}{\nu-5} - \dots - \frac{2r(2r-1)}{(\nu-4r-1)} \dots \right] ; \quad \nu = 2z^2 \quad . \quad (12b)$$

Convergence profile mappings were used to determine the number of terms necessary to obtain accuracy to five decimal places. Ellipses were then fitted to these profiles to ensure that an adequate number of terms was retained in the expansion for a given argument.

IV. INPUT PREPARATION

The first two cards contain 119 Alpha numeric characters in columns 2-72 (card 1) and 1-47 (card 2). Column 1, card 1 is left blank. Even if all the columns on card 1 or card 2 are blank, both cards must be present. In the program all isotopes with fission cross sections are to be listed first, and then the remainder. If this procedure is not followed, the absorption resonance integrals will be printed correctly but fission integrals will not. There are no other restrictions on the ordering of isotopic data.

The input is then:

card 1 }
card 2 } See above.

card 3: N, the number of subintervals per logarithmic decrement Δ .
 $0 < N \leq 100$. FORMAT, I3.

IP, the number of heavy isotopes. $0 < I \leq 4$. FORMAT, I3.

IFP, the number of fissionable isotopes, $0 < IFP \leq 4$. FORMAT, I3.

ICO, the number of subintervals per output statement,
 $0 < ICO \leq 1000$. FORMAT, I3.

EU, upper energy limit (ev). $0 < EU$. FORMAT, E12.6

EL, lower energy limit (ev). $0 < EL$. FORMAT, E12.6

AO, $4A/(A+1)^2$, A = heavy atom scattering mass (see text).
 $0 < AO$. FORMAT, E12.6

TEMP, heavy atom temperature, ev. $0 \leq T$. FORMAT, E12.6

SMOD, moderator scattering cross section (cm^{-1}). $0 < S \text{ MOD}$.
 FORMAT, E12.6

card 4: $J(1), \dots, J(IP)$ the number of resonance levels for isotopes 1, ..., IP.
 $0 < J \leq 75$. FORMAT, I12

card 5 to card 4 + IP; on each card:

AMAS, the atomic mass (amu) of isotope i

SW, the statistical weight $\left[\frac{2J+1}{2(2I+1)} \right]$ of isotope i

SIGPT, the potential scattering cross section (barns) of isotope i

ABUN, the density of nuclei of isotope i (per barn-cm), FORMAT,
 4E12.6

Card 4 + IP + 1 to card 4 + IP + $\sum_{L=1}^{IP} J(L)$ on each and for the Kth resonance
 of isotope L:

$ER(K,L)$, energy (ev)

$\Gamma_\gamma(K,L)$, gamma width (ev)

$\Gamma_n(K,L)$, neutron width (ev)

$\Gamma_f(K,L)$, fission width (ev)

FORMAT 3E12.6

(N.B.: The data on each card obviously must refer to the same level;
 and the first $J(1)$ cards must refer to isotope 1, the next $J(2)$
 to isotope 2, etc)

For use with the Argonne Monitor system, all input is put on tape
 (logical tape 7). To run problems sequentially, simply stack the data cards
 for the various problems in sequence. Each set of data must be complete
 in itself, and there should be no extra cards between data decks. Avoid the
 use of resonances at $ER(K,L) = 0$. This will cause a divide check; should
 there be an inaccurate level count, this can occur.

Table I

RESONANCE PARAMETERS (For problems discussed in text)

<u>Level Energy</u>	<u>Gamma Gamma</u>	<u>Gamma N</u>	<u>Gamma F</u>
<u>U^{235}</u>			
-0.140000E-01	0.330000E-01	0.282000E-02	0.194000E-00
-0.200000E-01	0.330000E-01	0.340000E-06	0.860000E-01
0.273000E-00	0.290000E-01	0.290000E-05	0.990000E-01
0.420000E-00	0.270000E-01	0.120000E-05	0.213000E-00
0.910000E+00	0.300000E-01	0.137000E-04	0.330000E-00
0.114000E+01	0.440000E-01	0.172000E-04	0.125000E-00
0.203500E+01	0.350000E-01	0.770000E-05	0.120000E-01
0.282000E+01	0.300000E-01	0.300000E-05	0.700000E-01
0.316000E+01	0.310000E-01	0.323000E-04	0.155000E-00
0.360000E+01	0.370000E-01	0.460000E-04	0.450000E-01
0.484000E+01	0.250000E-01	0.520000E-04	0.400000E-02
0.545000E+01	0.330000E-01	0.220000E-04	0.375000E-01
0.580000E+01	0.330000E-01	0.160000E-04	0.375000E-01
0.620000E+01	0.330000E-01	0.270000E-04	0.375000E-01
0.638000E+01	0.450000E-01	0.280000E-03	0.150000E-01
0.709000E+01	0.330000E-01	0.109000E-03	0.220000E-01
0.879000E+01	0.410000E-01	1.000000E-03	0.520000E-01
0.928000E+01	0.330000E-01	0.122000E-03	0.440000E-02
0.970000E+01	0.330000E-01	0.400000E-04	0.375000E-01
0.101600E+02	0.330000E-01	0.640000E-04	0.375000E-01
0.106400E+02	0.330000E-01	0.330000E-04	0.375000E-01
0.111100E+02	0.330000E-01	0.470000E-04	0.375000E-01
0.116400E+02	0.330000E-01	0.680000E-03	0.260000E-02
0.123800E+02	0.420000E-01	0.137000E-02	0.180000E-01
0.132600E+02	0.330000E-01	0.990000E-03	0.375000E-01
0.138000E+02	0.330000E-01	0.150000E-03	0.375000E-01
0.141000E+02	0.330000E-01	0.200000E-03	0.375000E-01
0.145300E+02	0.330000E-01	0.15 E-03	0.4 E-01
<u>U^{238}</u>			
0.668 E+02	0.25 E-01	0.148 E-02	
0.102 E+02	0.246 E-01	0.140 E-05	
0.21 E+02	0.25 E-01	0.900 E-02	
<u>Au^{197}</u>			
0.4906 E+01	0.125 E-00	0.156 E-01	

V. OUTPUT

Since the program is compiled to run on the Argonne Monitor system, all output is on tape 6. (Tape 2 is used as a scratch tape.)

The first page of output includes the problem identification (cards 1 and 2) and the input data on card 3. The rest of the input data, for each isotope in turn, are printed on the next pages. Each isotope starts a new page.

Following this are sheets labeled alternately: "Resonance Integral, Fission" with columns labeled ENERGY, COLLISION DENSITY, FLUX, RESINT ISOTOPE 1, etc. (Recall that the term "FLUX" is a misnomer since the quantity in question is just the energy times the collision density.) The entries on each page correspond to the quantities calculated during one major cycle of the code, 10N lethargy steps.

A typical code listing is given in Appendix A. Since the code is experimental, this listing is not necessarily the one in current use, but all the vital features of the code are present. Possible changes in the code are discussed in the next section.

VI. EARLY RESULTS AND PROGRAM OF FUTURE WORK

Results

An interesting case to study is a low-enrichment, high-conversion lattice. We took as an example a mixture of water and uranium in equal volumes. (The effects of rod size were neglected at this point.) The temperature was taken as 0°K and the heavy atom scattering mass was 238. Three U²³⁵ enrichments were studied: 1, 2, and 3 per cent. In addition, gold at 10⁻⁶ atom/(b-cm) was included to study the response of a typical monitor foil.

Resonance parameters are given in Table I; the U²³⁵ data were taken from Harvey⁽³⁾ and WCAP-1434⁽⁴⁾, whereas the data for U²³⁸ and gold come from BNL-325⁽⁵⁾.

We used a version of the code which calculated the real fluxes, and these are plotted, for 1% enrichment, in Fig. I. Also shown on Fig. I by means of dashed lines are the changes in the flux when calculated for 3% enrichment. The flux perturbations from the various resonances are clearly seen. Also to be noted are the effects of the 6.68-ev U²³⁸ resonance and the 4.84-ev U²³⁵ resonance on the gold resonance at 4.91 ev. The gold resonance integral over the energy range indicated is given in Table II for the various enrichments. The shielding mostly comes from U²³⁸, but there is a small U²³⁵ effect.

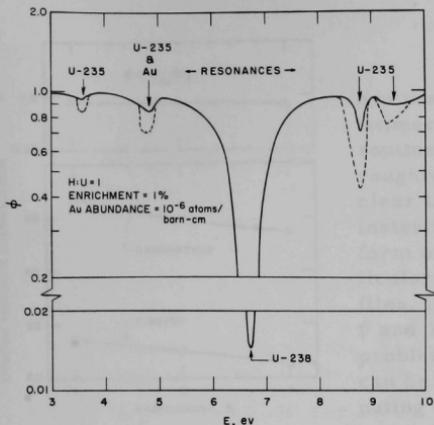


Table II

RESONANCE INTEGRAL OF DILUTE GOLD
IN H:U = 1 MIXTURE.
ENERGY RANGE 3 - 10 ev.

Enrichment, %	Integral (b)
1	1357
2	1337
3	1333

(Resonance integral over this energy range,
1/E spectrum: 1445.)

Figure II shows graphs of the U^{235} resonance integrals as a function of enrichment. Based on moderator scattering per U^{235} atom, a larger variation in the cross section as well as a larger cross section would be expected. The U^{238} dominates the spectrum and suppresses the scattering effect. The shielding by the U^{238} amounts to about 20% of the cross section effect [see, e.g., the tabulation in Resonance Integral Newsletter No. 8(6)]. The ratio of capture to fission in U^{235} , α , also shown in Fig. II, is practically independent of enrichment.

For check purposes, infinite dilution integrals were calculated through use of small abundances, and these were checked against results obtained by use of the code RE-266,(7) a code designed especially for computing infinite dilution integrals. For U^{235} , agreement was better than 0.1%.

Future Program

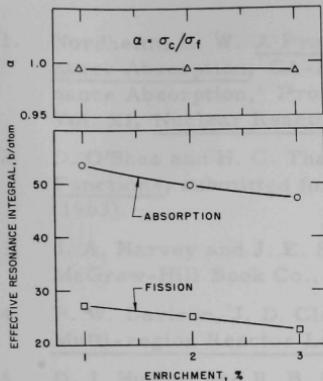


Fig. II. Effective Resonance Integrals of U^{235} in $H/U = 1$ Mixture; and α of U^{235}

integral from 3 to 10 ev. Since some levels in the range 0-3 ev contribute much less than 2 b, mere displacement along the energy scale is not a good test. A test of $\sigma_0/(1+x^2)$ is not a time saver.

For the present, we make a survey of a problem by taking an actual decimal dump of a typical problem and examining the cross-section contributions PP SIGA, PP SIGH from each level. Levels whose contribution is small may then be removed from the data deck and the full problem run.

The use of a uniform mesh is clearly wasteful; a variable mesh spacing would help. In this case, small resonances or the resonance capture in elements of low abundance would have to be calculated analytically in regions of large mesh spacing.

The investigation of these points together with such obvious topics as inclusion of unresolved resonances, effects of lumping, differences in scattering mass, and exact moderator effect forms an ambitious program of work.

The code is too slow. Future work has the main task of speeding the code. At temperatures other than 0°K, the W subroutine requires about 8 ms per entry and roughly triples the running time. It is not clear that a faster W subroutine exists; instead, it may prove useful to change the form of access to the W routine. In particular, with a larger machine with disc files, it will probably save time to enter the ψ and χ functions as a table for a given problem and refer to that. Some small gain can be made by changing the order of computing σ_0 , etc.; the main difficulty however, comes from the attempt to compute a sum over all levels.

It is not clear how to eliminate levels in a systematic way. The -1.4-ev level in U^{235} contributes about 2 b to the resonance

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ACKNOWLEDGEMENT

I wish to acknowledge the patient and helpful assistance given me by Mrs. D. Bingaman and other members of the Applied Mathematics Division. Messrs. Paul J. Persiani and A. E. McCarthy were helpful in the selection of the U²³⁵ negative energy parameters and the calculation of resonance integrals at infinite dilution.

APPENDIX A

Typical Fortran Listing for 1559/RE

# 004	3/7/63	MEYER, L.	1559/RE	3627 *** 6296
0307631503	C KELBER	44111-051111559RE	704Z0	
\$COMPILE			3 03 RM	3/7/63 1559

C 1559/RE.GEAR FOUR. A PROGRAM TO COMPUTE THE RESONANCE INTEGRALS
C FOR UP TO FOUR ISOTOPES WITH AS MANY AS 75 LEVELS EACH.
C PLEASE RETURN ALL RESULTS TO C.N.KELBER,D-208.
DIMENSION(1000),TPSIGA(4),TPSIGH(4),TPSIGS(4),
XJ(4),GAMT(75,4),GG(75,4),GN(75,4),GF(75,4),ZETA(75,4),AMAS(4),
XEX(75,4),ER(75,4),PSY(75,4),CHY(75,4),SIGO(75,4),SW(4),ABUN(4),
XPPSIGA(75,4),PPSIGH(75,4),PPSIGS(75,4),SIGPT(4),
X PRAT(1000,4),PRFT(1000,4),A(1000),G(101),H(101),
XAJ(1000),F(1000),PHY(1000),RESINT(1000,4),P(20),Z(5)
DIMENSIONASTART(4),FSTART(4)

SAN	ALF	N
-----	-----	---

SAIP	ALF	IP
------	-----	----

SAEU	ALF	EU
------	-----	----

SAEL	ALF	EL
------	-----	----

SAAO	ALF	AO
------	-----	----

SAATE	ALF	TEMP
-------	-----	------

SASMO	ALF	SMOD
-------	-----	------

1 FORMAT(12A6)

2 FORMAT(4I3,5E12.6)

3 FORMAT(1I12)

4 FORMAT(4E12.6)

410 READINPUTTAPE7,1,(P(IA),IA=1,20)

READINPUTTAPE7,2,N,IP,IFP,ICOUNT,EU,EL,AO,TEMP,SMOD

READINPUTTAPE7,3,(J(L),L=1,IP)

READINPUTTAPE7,4,(AMAS(L),SW(L),SIGPT(L),ABUN(L),L=1,IP)

D05L=1,IP

JL=J(L)

5 READINPUTTAPE7,4,(ER(K,L),GG(K,L),GN(K,L),GF(K,L),K=1,JL)

6 FORMAT(1H1/1H0/1H0/1H0/1H0/)

X94H 1559 RE A PROGRAM TO COMPUTE THE EFFECTS OF

XINTERFERENCE BETWEEN RESONANCES///

PROBLEM IDENTIFICATION//

X)

7 FORMAT(2U6)

WRITEOUTPUTTAPE6,6

WRITEOUTPUTTAPE6,7,(P(IA),IA=1,20)

8 FORMAT(1H1/1H0/1H0/

INPUT DAT

X64H

XA//)

9 FORMAT(65H

FOR THIS

X PROBLEM,//43H THE LOGARITHMIC DECREMENT IS DIVIDED INTO 13,21H IN

X INTERVALS. THERE ARE 13,14H ISOTOPES, AND 13,17H OF THEM FISSION.//)

10 FORMAT(20H THE UPPER ENERGY ISE12.5,17H EV.,THE LOWER ISE12.5,35H

XEV. HEAVY ATOM SCATTERING ALPHA ISE12.5//26H THE TEMPERATURE IN EV

X. ISE12.5,28H THE MODERATOR SCATTERING ISE12.5,8H PER CM.///)

RESULTS ARE PRINTED A

11 FORMAT(7H

XT INTERVALS OF 13,16H LETHARGY STEPS.//)

WRITEOUTPUTTAPE6,9,N,IP,IFP

WRITEOUTPUTTAPE6,10,EU,EL,AC,TEMP,SMOD

WRITEOUTPUTTAPE6,11,ICOUNT

C IN CASE OF INPUT ERROR

12 FORMAT(32H INPUT ERROR. SEE ON LINE PRINT.)

C TEST INPUT

13 FORMAT(7H ERROR.A6,31H OUT OF RANGE.RETURN TO SENDER./)

ATEMP=TEMP+1.E-9

II=0

14 IF(N)15,15,17


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15 WRITEOUTPUTTAPE6,12
16 PRINT13,AN
17 II=1
18 IF(IP)18,18,20
19 WRITEOUTPUTTAPE6,12
20 PRINT13,AIP
21 II=1
22 IF(100-N)21,24,24
23 WRITEOUTPUTTAPE6,12
24 PRINT13,AN
25 II=1
26 EQUIVALENCE(Z(1),EU),(Z(2),EL),(Z(3),AO),(Z(4),ATEMP),
   X(Z(5),SMOD)
27 D034J=1,5
28 IF(Z(J))26,26,34
29 WRITEOUTPUTTAPE6,12
30 GO TO(29,30,31,32,33),J
31 PRINT13,AEU
32 II=1
33 GO TO 34
34 PRINT13,AEL
35 II=1
36 GO TO 34
37 PRINT13,AAO
38 II=1
39 GO TO 34
40 PRINT13,AATE
41 II=1
42 GO TO 34
43 PRINT13,ASMOD
44 II=1
45 GO TO 34
46 CONTINUE
47 IF(II-1)37,36,36
48 GOTO410
49 GOTO40G
C READ OUT ISOTOPE DATA
50 FORMAT(1H1//,6TH) IN
51 FORMAT(25H THIS ISOTOPE HAS14,8H LEVELS.//)
52 FORMAT(21H ATOMIC MASS=E12.6,12H STAT.WT.=E12.6,
   X13H POT.SCAT.=E12.6,13H ABUNDANCE=E12.6//)
53 FORMAT(80H LEVEL ENERGY GAMMA GAMMA GAMM
   XMA N GAMMA F//)
54 FORMAT(4E20.6)
55 D046L=1,IP
56 WRITEOUTPUTTAPE6,50,L
57 WRITEOUTPUTTAPE6,51,J(L)
58 WRITEOUTPUTTAPE6,52,AMAS(L),SW(L),SIGPT(L),ABUN(L)
59 WRITEOUTPUTTAPE6,53
60 JL=J(L)
61 WRITEOUTPUTTAPE6,54,(ER(K,L),GG(K,L),GN(K,L),
   XGF(K,L),K=1,JL)
62 GOTO70
63 TSIGPT=0.
64 D072L=1,IP
65 TSIGPT=TSIGPT+SIGPT(L)*ABUN(L)
66 D=LOGF(1./(1.-AO))/FLOAT(F(N))
67 IMAX=10*N
68 GOT080
C AFTER THE INPUT HAS BEEN READ IN WE GET SET.
69 IB=0

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81 E1=EU
82 D083J=1,IP
83 ASTART(J)=0.
84 D085J=1,IFP
85 FSTART(J)=0.
GOTO9C
90 CONTINUE
91 REWIND2
92 REWIND3
93 REWIND4
95 D011UI=1,IMAX
PSIGA=0.
PSIGS=0.
96 U=FLOATF(I)*D
E(I)=E1/EXPF(U)
D0105L=1,IP
TPSIGA(L)=0.
TPSIGH(L)=0.
TPSIGS(L)=0.
JL=J(L)
D0100K=1,JL
GAMT(K,L)=GG(K,L)+GN(K,L)+GF(K,L)
597 IF(TEMP>598,.598,.98 XGAMT
598 EX(K,L)=2.* (E(I)-ER(K,L))/GAMT(K,L)
599 PSY(K,L)=1./ (1.+EX(K,L)**2)
600 CHY(K,L)=2.*EX(K,L)/(1.+EX(K,L)**2)
GOTO99
98 ZETA(K,L)=SQRTF((AMAS(L)*GAMT(K,L)**2)/(4.*E(I)*TEMP))
EX(K,L)=2.* (E(I)-ER(K,L))/GAMT(K,L)
CALLW(ZETA(K,L)+EX(K,L)/2.,ZETA(K,L)/2.,REW,AIMW)
PSY(K,L)=ZETA(K,L)*.8862265*REW
CHY(K,L)=ZETA(K,L)*1.772453*AIMW
99 SIGO(K,L)=(2.62E+6)*SW(L)*GN(K,L)/(ABSF(ER(K,L))*GAMT(K,L))
PPSIGA(K,L)=(GG(K,L)+GF(K,L))*SIGO(K,L)*PSY(K,L)
X*SQRTF(ABSF(ER(K,L))/E(I))/GAMT(K,L)
PPSIGH(K,L)=GF(K,L)*PPSIGA(K,L)/(GG(K,L)+GF(K,L))
TPSIGA(L)=TPSIGA(L)+ABUN(L)*PPSIGA(K,L)
TPSIGH(L)=TPSIGH(L)+ABUN(L)*PPSIGH(K,L)
PPSIGS(K,L)=(GN(K,L)*SIGO(K,L)*PSY(K,L)/GAMT(K,L))+XSQRTF(SIGPT(L)*SIGO(K,L)*SW(L)*GN(K,L)/GAMT(K,L))*CHY(K,L)
100 TPSIGS(L)=TPSIGS(L)+ABUN(L)*PPSIGS(K,L) END K
PSIGA=PSIGA+TPSIGA(L)
105 PSIGS=PSIGS+TPSIGS(L)
106 D0109L=1,IP
PRAT(I,L)=TPSIGA(L)/(PSIGS+PSIGA+TSIGPT+SMOD)
109 PRFT(I,L)=TPSIGH(L)/(PSIGS+PSIGA+TSIGPT+SMOD)
110 A(I)=(PSIGS+TSIGPT)/((PSIGS+TSIGPT+PSIGA+SMOD)*AO)
GOTO120
C PREPARE TO GENERATE FLUXES
120 IF(IB>0,125,200
C IF IB IS ZERO WE GENERATE SOME STARTING FLUXES
C THE ASYMPTOTIC VALUES ARE USED
125 MN=N+1
D0130J=1,MN
AD=FLOATF(N+1)*D
EUU=EU*EXPF(AD)
UU=FLOATF(J)*D
AE=EUU/EXPF(UU)
G(J)=(TSIGPT+SMOD)/AE
130 H(J)=TSIGPT/(AO*(TSIGPT+SMOD))
131 WRITETAPE2,(G(J),J=1,MN)
WRITETAPE2,(H(J),J=1,MN)

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ENDFILE2
REWIND2
132 FF=G(N+1)
AA=H(N+1)
AAJ=(TSIGPT/(EU*D))-.5*FF*AA
GOT020
C NOW WE GO INTO THE ITERATION ROUTING
C CALCULATE F(I) AND PHY(I)
200 WRITEOUTPUTTAPE6,202
202 FORMAT(1H1/85H
X RESONANCE INTEGRALS,ABSORPTION//119H ENERGY COLLISION
XDENSITY FLUX RESINT ISOTOPE 1 RESINT ISOTOPE 2 RESINT
XISOTOPE 3 RESINT ISOTOPE 4//)
201 MN=N+1
READTAPE2,(G(I),I=1,MN)
READTAPE2,(H(I),I=1,MN)
AJ(I)=AAJ-.5*(G(I)+H(I)+G(2)*H(2))+FF*AA
F(I)=(D*AJ(I)+(SMOD/E(I)))/(1.-.5*D*A(I))
REWIND2
205 D0220I=2,IMAX
NN=N+2
IF(I>NN)210,215,215
210 AJ(I)=AJ(I-1)-.5*(G(I)*H(I)+G(I+1)*H(I+1))
X+F(I-1)*A(I-1)
F(I)=(D*AJ(I)+(SMOD/E(I)))/(1.-.5*D*A(I))
PHY(I)=F(I)*E(I)
GOT0220
215 NI=I-N
216 AJ(I)=AJ(I-1)-.5*(F(NI-1)*A(NI-1)+F(NI)*A(NI))
X+F(I-1)*A(I-1)
217 F(I)=(D*AJ(I)+(SMOD/E(I)))/(1.-.5*D*A(I))
218 PHY(I)=E(I)*F(I)
GOT0220
220 CONTINUE
J=IMAX-N-1
WRIETAPE2,(F(I),I=J,IMAX)
WRIETAPE2,(A(I),I=J,IMAX)
ENDFILE2
REWIND2
C TAPE 2 IS NOW READY FOR THE NEXT TIME THRU.
C SET THE AUXILLARY CONSTANTS
AAJ=AJ(IMAX)
FF=F(IMAX)
AA=A(IMAX)
GOT0230
C NOW START THE EDIT ROUTINE
230 D0240L=1,IP
RESINT(I,I)=ASTART(I) SEE 230
232 D0240I=2,IMAX
235 RESINT(I,I)=RESINT(I-1,I)+.5*D*(PHY(I)*PRAT(I,I)
X+PHY(I-1)*PRAT(I-1,I))
240 CONTINUE
GOT0240
242 IF(IP-1)243,243,247
243 D0245I=1,IMAX
RESINT(I,2)=0.
RESINT(I,3)=0.
245 RESINT(I,4)=0.
GOT0255
247 IF(IP-2)255,248,250
248 D0249I=1,IMAX

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249 RESINT(I,3)=0.
250 GOT0255
251 IF(IP=3)255,251,255
252 DO252I=1,IMAX
253 RESINT(I,4)=0.
254 GOT0255
255 ICON=0
256 DO260 I=1,IMAX
ICON=ICON+1
IF(ICON-ICOUNT)260,257,260
257 WRITEOUTPUTTAPE6,265,(E(I),F(I),PHY(I),
XRESINT(I,1),RESINT(I,2),RESINT(I,3),RESINT(I,4))
ICON=0
258 CONTINUE
265 FORMAT(7E17.5)
GOT0465
465 DO466J=1,IP
466 ASTART(J)=RESINT(IMAX,J)
GOT0266
266 IF(IFP)270,350,270
270 WRITEOUTPUTTAPE6,272
272 FORMAT(1H1/82H
X RESONANCE INTEGRALS,FISSION//119H ENERGY COLLISION DEN
XSITY FLUX RESINT ISOTOPE 1 RESINT ISOTOPE 2 RESINT ISO
XTOPE 3 RESINT ISOTOPE 4//)
GOT0280
280 D0290L=1,IFP
SEE 265

RESINT(I,I)=FSTART(I)
282 D0290I=2,IMAX
285 RESINT(I,I)=RESINT(I-1,I)+.5*D*(PHY(I)*PRFT(I,I)
X+PHY(I-1)*PRFT(I-1,I))
290 CONTINUE
292 IF(IFP-1)293,293,297
293 D0295I=1,IMAX
RESINT(I,2)=0.
RESINT(I,3)=0.
295 RESINT(I,4)=0.
GOT0313
297 IF(IFP-2)303,298,300
298 D0299I=1,IMAX
RESINT(I,3)=0.
299 RESINT(I,4)=0.
300 IF(IFP-3)303,301,303
301 D0302I=1,IMAX
302 RESINT(I,4)=0.
GOT0313
303 ICON=0
304 D0310I=1,IMAX
ICON=ICON+1
IF(ICON-ICOUNT)310,305,310
305 WRITEOUTPUTTAPE6,265,(E(I),F(I),PHY(I),
XRESINT(I,1),RESINT(I,2),RESINT(I,3),RESINT(I,4))
ICON=0
310 CONTINUE
311 D0312J=1,IFP
312 FSTART(J)=RESINT(IMAX,J)
GOT0350
350 FE=E(IMAX)
351 IF(FE-EL)400,400,380
380 IB=IB+1
GOT0385
385 E1=FE
GOT090
C START OVER AGAIN
400 WRITEOUTPUTTAPE6,405
GOT0414
405 FORMAT(1H1/34H THIS PROBLEM IS COMPLETE.)
END ( 1 , 1 , 0 , 1 , 0 )
ANL-30

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